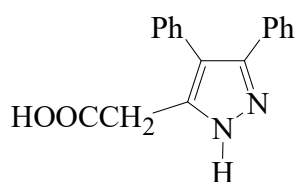




>>Entry Name: 3,4-Diphenyl-1*H*-pyrazole-5-acetic acid, 9Cl



Related CAS Registry Numbers(s): 78218-49-2

Molecular Formula: C₁₇H₁₄N₂O₂

Molecular Weight: 278.31

Accurate Mass: 278.105528

Percentage Composition: C 73.37%; H 5.07%; N 10.07%; O 11.50%

>>Derivative: Na salt

Hazard & Toxicity: LD₅₀ (rat, orl) 13 mg/kg

>>Derivative: 1-(2-Methylpropyl)

Synonym(s): Bufeazolac, INN. LM 22070

CAS Registry Number: 50270-32-1

Type of Compound Code(s): XA0660 XA1700 XA2150

Molecular Formula: C₂₁H₂₂N₂O₂

Molecular Weight: 334.417

Accurate Mass: 334.168128

Percentage Composition: C 75.42%; H 6.63%; N 8.38%; O 9.57%

Use/Importance: Analgesic, antiinflammatory, antipyretic agent

Physical Description: Cryst. (MeCN)

Melting Point: Mp 181°

Calculated Log P Data: Log P 4.97 (calc)

>>Derivative: 1-Ph

Synonym(s): 1,3,4-Triphenyl-1*H*-pyrazole-5-acetic acid, 9Cl. **Isofezolac**, INN. Sofenac. LM22102

CAS Registry Number: 50270-33-2

Type of Compound Code(s): XA0660 XA1700 XA2150

Molecular Formula: C₂₃H₁₈N₂O₂

Molecular Weight: 354.407

Accurate Mass: 354.136828

Percentage Composition: C 77.95%; H 5.12%; N 7.90%; O 9.03%

Use/Importance: Analgesic, antipyretic, antiinflammatory agent

Development Status: Launched 1984

References:

Ger. Pat., 1973, *Sogeras*, 2 312 256; *CA*, **79**, 146516a, (*synth, pharmacol*)

Mizoule, J. *et al.*, *Arch. Int. Pharmacodyn. Ther.*, 1979, **238**, 305, (*pharmacol, tox*)

Bannier, A. *et al.*, *J. Chromatogr.*, 1980, **182**, 369; 1982, **227**, 213, (*hplc*)

Martindale, The Extra Pharmacopoeia, 30th edn., *Pharmaceutical Press*, 1993, 16863